

Antiferromagnetism in the 2D Hubbard Model – Phase Transition and Local Quantities

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Abstract

We present a first study of the antiferromagnetic state in the $2D$ U - t - t' model at finite temperatures by the composite operator method, providing simultaneously a fully self-consistent treatment of the paramagnetic and the AF phase. Near half filling the critical value of the Coulomb repulsion as a function of t' and the temperature dependence of the magnetization and internal energy have been studied.

Keywords: Hubbard Model; Strongly Correlated Electron Systems; Antiferromagnetism; Composite Operator Method

1. Introduction

An antiferromagnetic phase is observed in most *cuprate* high T_c superconductors. On the other hand antiferromagnetic correlations are considered to play an important role in the mechanism of pair formation in those materials.

The normal phase of $2D$ Hubbard model has been studied intensively by the composite operator method (COM), leading to good agreement with numerical results and experimental data [1]. A study of the AF phase in the $2D$ Hubbard model by COM is therefore supposed to give some insight in both, the nature of antiferromagnetism and the pair forming mechanism.

2. Results

We investigate the Hubbard Hamiltonian on a $2D$ square lattice with additional next-nearest neighbor hopping t'

$$H = \sum_{i,j,\sigma} (t_{ij} + t'_{ij} - \delta_{ij}\mu) c_{\sigma}^{\dagger}(i) c_{\sigma}(j) + U \sum_i n_{\uparrow}(i) n_{\downarrow}(i)$$

by means of COM [1], using the Hubbard operators $\xi_{\sigma}(i) = c_{\sigma}(i) (1 - n_{\bar{\sigma}}(i))$ and $\eta_{\sigma}(i) = c_{\sigma}(i) n_{\bar{\sigma}}(i)$ as components of the basic spinor $\Psi(i)$.

To describe the AF phase we introduce a coarse grained, bipartite lattice with lattice constant a , overlaying the chemical lattice by grouping together pairs of nearest neighbors in the usual way. For the two sublattices A and B we assume a symmetric electronic state, $\langle A, \sigma \rangle = \langle B, \bar{\sigma} \rangle$.

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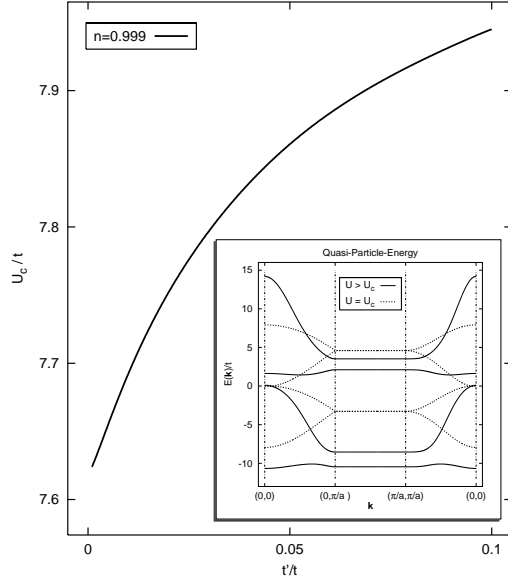


Fig. 1. Critical Coulomb interaction at which the sublattice magnetization vanishes as a function of the next-nearest neighbor hopping t' at $k_B T = 0.01t$ and $n = 0.999$. As inset the band structure is shown for U_c and $U > U_c$ at the same temperature and particle density.

The retarded Greens functions $G^{XY}(\mathbf{k}, \omega) = \langle \{ \Psi^\dagger(i), \Psi(j) \} \rangle_{F.T.}$ with $X, Y \in \{A, B\}$ in the static approximation where finite life time effects are neglected are determined in a fully self-consistent way by the constraints $\langle \xi_\sigma(i) \eta_\sigma^\dagger(i) \rangle = 0$ and $\langle \xi_\uparrow(i) \xi_\uparrow^\dagger(i) \rangle = \langle \xi_\downarrow(i) \xi_\downarrow^\dagger(i) \rangle$, emerging from the algebra of the Hubbard operators, namely from the Pauli principle.

The critical value of the Coulomb interaction is given in Fig. 1 as function of t' . U_c turns out to be significantly larger than in results obtained by renormalization group techniques [2][3], which might be due to the fact, that the latter is valid only in the weak coupling limit, whereas COM provides a good approximation for intermediate and strong coupling as well. The band structure shows the opening of a gap at the transition line between the paramagnetic and the AF phase.

In Fig. 2 the sublattice magnetization $m = n_\uparrow^A(i) - n_\downarrow^A(i)$ is plotted versus temperature for different values of the Coulomb interaction. With de-

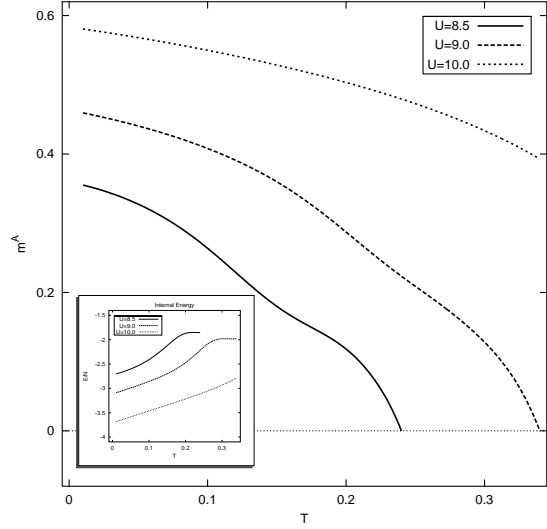


Fig. 2. Sublattice magnetization as a function of temperature for various values of U at $k_B T = 0.01t$, $t' = 0.05t$ and $n = 0.999$. As inset the corresponding values of the internal energy per site are plotted.

creasing magnetization the energy per site, which is not sublattice dependent because of the above symmetry assumption on the electronic state, is increasing, reaching finally the paramagnetic value at vanishing m .

3. Conclusions

First results for the AF phase of the 2D Hubbard model obtained by COM within a fully self-consistent treatment were presented. Further results and a detailed elaboration of the theoretical framework will be presented elsewhere.

References

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